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Stopping Power Theory

Particles with mass are brought to rest, or stopped, inside a target medium while photons are absorbed. This observation lead to the formulation of a theoretical framework for stopping power. The scope of this problem quickly becomes large as one considers the variety of beam species, which span the periodic table, as well as stopping media. This multiplicity is compounded by the broad range of interesting projectile kinetic energies that vary over 12 orders of magnitude of electron volts. In terms of target diversity, even a modest sample of compounds and alloys yields about 10^6 combinations of interest, making it impractical to provide measurements for all possible permutations [Sigmund, 1998]. So, while theory is essential, it can by no means be complete without the incorporation of experimental data to augment it. Knowledge of stopping power is needed in a wide range of disciplines, including radiation medicine and therapy, radiation detection, cosmic ray research, particle accelerator design, radiation safety, and many others.

A charged particle of rest mass significantly larger than that of an electron is considered to be a "heavy" charged particle. This includes mesons, protons, α-particles, and heavier nuclei with $Z \geq 3$. Electrons and positrons are considered "light" charged particles. The electromagnetic interaction of heavy charged particles with the electrons in matter is described by the Bethe-Bloch stopping power formula [Bethe, 1930; Bloch, 1933]:

$$-\frac{dT}{dx} = \frac{nz^2e^4}{4\pi\epsilon_0^2 m_\mathrm{e} v^2} L_\mathrm{o}. \tag{1}$$

The variables in Equation (1) have the following meanings: $n = N_\mathrm{A} Z\rho/A$ is the electron density of the target, with N_A the Avogadro number and Z, A, and ρ the atomic number, atomic mass, and mass density of the target, respectively; z is the atomic number of the projectile; e is the charge of the electron; ϵ_o is the permittivity of free space; m_e is the rest mass of the electron. The factor L_o in

Equation (1) is referred to as the stopping logarithm (sometimes called the stopping number), and is a collection of logarithmic terms plus some extra corrections. At least outside the field of high energy physics, the unit of Equation (1) is commonly given as keV/μm.

The basic form of L_0 takes two forms. The form due to Niels Bohr, $L_0 = \ln(Cm_e v^3/ze^2\omega)$, is the result of a classical derivation, with $C = 1.1229$ and $\omega = I/\hbar$ [Bohr, 1913; Bohr, 1915]. Alternatively, the form $L_0 = \ln(2m_e v^2/I)$ is attributed to Hans Bethe [Bethe, 1930]. I is the mean ionization potential of the target in units of eV and characterizes the rate of energy loss per unit path length. The mean ionization potential is difficult to calculate, so, in practice, the best values of I are obtained through measurement. These logarithms meet at Bohr's κ parameter of $\kappa = 2zv_0/v \cong 1$, with $v_0 = e^2/\hbar$ the Bohr velocity. Below κ, or at lower projectile velocities, the impact parameter for Coulomb scattering, $b = 2ze^2/mv^2$, is greater than the de Broglie wavelength, $\lambda/2\pi = \hbar/mv$, meaning that the projectile behaves classically, or particle-like. Above κ, or at higher projectile velocities, the converse is true and the projectile behaves quantum mechanically, or wave-like. Equation (1) can be rewritten in a form that follows Hans Bethe's and Felix Bloch's derivation using quantum perturbation theory:

$$-\frac{dT}{dx} = \frac{nz^2e^4}{4\pi\epsilon_0^2 m_e v^2}\left[\ln\left(\frac{2m_e v^2}{I}\right) - \ln\left(1 - \frac{v^2}{c^2}\right) - \frac{v^2}{c^2} - \frac{\delta}{2}\right], \tag{2}$$

where c is the speed of light in vacuum. The standard relativistic corrections $-\ln(1 - v^2/c^2) - v^2/c^2$ become important when the projectile is moving with a velocity that is a significant fraction of the speed of light [Bohr, 1913; Bohr, 1915; Fano, 1963]. In other words, $L_0 \cong \ln(2m_e v^2/I)$ when the velocity of the projectile is small compared to the speed of light. The first three terms in the stopping logarithm of Equation (2) are typically called the Bethe result [Weaver and Westphal, 2002]. The last term, $-\delta/2$, is the density effect correction.

Equation (2) describes the kinetic energy transferred to the surrounding medium per unit path length (hence the minus sign) when a charged particle traverses matter. In medical physics and radiation protection, Equation (2), which represents the primary mode of energy loss for charged particle passage through matter, is often referred to as the LET and is commonly written as dE/dx instead of $-dT/dx$. Because these electrons receive energy from the projectile, they can be ionized, or freed from their atomic orbitals. Ionization of electrons by the passage of a charged particle through the sensitive volume of a detector is the primary mechanism used by most detectors to register charged particles and energetic photons. Equation (2) assumes that the electron is "free," or not bound. This assumption is valid since the energy required to bind an electron to a nucleus is likely to be very small relative to the kinetic energy of the incident charged particle.

In order to accurately calculate the stopping power of a charged particle passing through matter, one must consider more corrections to the stopping logarithm of the Bethe-Bloch formula: $L_0 + \Delta L$. These additional considerations take into account other kinetic energy dependent phenomena described below.

Density Effect Correction

The density effect correction, which is important to the stopping power phenomenon called the relativistic rise, represents the reduction of the collision stopping power due to the polarization of the medium caused by the passage of the incident charged particle. In dense targets, the field which perturbs electrons far from the projectile track is modified by the dielectric polarization of the atoms between those distant electrons and the projectile [Fermi, 1940; Sternheimer and Peierls, 1971]. At high energies, the density effect correction has the form:

$$-\frac{\delta}{2} = -\ln(\beta\gamma) + \ln\left(\frac{I}{\hbar\omega_{\mathrm{p}}}\right) + \frac{1}{2}, \tag{3}$$

where $\beta = v/c$, $\gamma = 1/\sqrt{1 - v^2/c^2}$, $\hbar = h/2\pi$ is the reduced Planck constant, and ω_{p} is the plasma frequency of the medium. For a neutral target medium consisting of a distribution of positively charged ions and negatively charged electrons, a displacement of the electrons with respect to the ions will result in a restoring Coulomb force. This restoration force drives the charge density to oscillate with a frequency equal to the plasma frequency. The density effect reduces the relativistic rise from $\sim \ln \gamma^2$ to $\sim \ln \gamma$. At intermediate energies, a parameterization of the density effect can be implemented [Sternheimer and Peierls, 1971]:

$$-\frac{\delta}{2} = -\frac{\delta_{\mathrm{high}}}{2} - \frac{a}{2}(X_1 - X)^m, \tag{4}$$

for $X_0 < X < X_1$. In Equation (4), $-\delta_{\mathrm{high}}/2$ is obtained from Equation (3), and X_0, X_1, a, and m are the Sternheimer density effect parameters [Sternheimer et al., 1984]. A computer program, given in Appendix A, has been written to compute the density effect parameters, including the mean ionization potential, for an arbitrary compound or mixture for which the molecular formula and density of the substance is known [Seltzer and Berger, 1982]. A low energy density effect correction specific to conductors exists and is given by [Sternheimer and Peierls, 1971]:

$$-\frac{\delta}{2} = -\frac{1}{2}\delta(X_0)10^{2(X-X_0)}, \tag{5}$$

for $X \leq X_0$, where $\delta(X_0) = 0$ for insulators; otherwise it is approximately equal to 0.1.

Electron Capture

Electron capture is manifest as a decrease in the projectile charge such that the bare nuclear charge, z, is replaced by the effective projectile charge, z^*, which is a function of its velocity v. For kinetic energies much greater than 1 GeV/n, $z^* \cong z$. For lower energies, the following empirical formula is useful [Pierce and Blann, 1968]:

$$z^* = z\left(1 - \exp\left\{-\frac{0.95\beta}{\alpha z^{2/3}}\right\}\right). \tag{6}$$

However, it has been shown experimentally that z^* depends on the atomic number of the target material, Z [Anthony and Lanford, 1982]:

$$z^* = z\left(1 - \mathrm{A}(Z)\exp\left\{-\frac{\mathrm{B}(Z)\beta}{\alpha z^{2/3}}\right\}\right), \tag{7}$$

with $\mathrm{A}(Z) = 1.16 - 1.91 \times 10^{-3}Z + 1.26 \times 10^{-5}Z^2$ and $\mathrm{B}(Z) = 1.18 - 7.5 \times 10^{-3}Z + 4.53 \times 10^{-5}Z^2$. A more recent analysis of a substantial energy loss and range dataset yields the formula [Hubert et al., 1989; Hubert et al., 1990]:

$$z^* = z(1 - x_1\exp\{-x_2 E^{x_3} z^{-x_4}\}). \tag{8}$$

In Equation (8), E is the kinetic energy of the projectile in MeV/n. For most target substances, $x_1 = \mathrm{C} + \mathrm{De}^{-\mathrm{E}z}$, with $\mathrm{C} = 1.164 + 0.2319\mathrm{e}^{-0.004302Z}$, $\mathrm{D} = 1.658$, and $\mathrm{E} = 0.05170$. Additionally, $x_2 = 8.144 + 0.09876\ln Z$, $x_3 = 0.3140 + 0.01072\ln Z$, and $x_4 = 0.5218 + 0.02521\ln Z$. Special-case effective charge parameters are specified in Table 1.

Table 1 Effective charge parameters for beryllium and carbon targets.

Target	x_2	x_3	x_4	**C**	**D**	**E**
Be	7.000	0.2643	0.4171	2.045	2.000	0.04369
C	6.933	0.2433	0.3969	2.584	1.910	0.03958

Shell Corrections

Shell corrections arise when the velocity of the projectile is comparable to the velocities of the electrons in the target atoms. These corrections address the following situations:

1. The velocity of the projectile is low enough such that the inner shell electrons of the target atom have velocities comparable to the projectile
2. The inner shell electrons have relativistic velocities for sufficiently heavy target atoms

The shell correction applicable to the first situation is [Fano, 1963]:

$$\Delta L_{\mathrm{shell}} = -\frac{\mathrm{C}}{Z}. \tag{9}$$

The function C in Equation (9) is given by [Bichsel, 1972]:

$$\begin{aligned} \mathrm{C} = {} & (4.22377 \times 10^{-7}\beta^{-2}\gamma^{-2} + 3.04043 \times 10^{-8}\beta^{-4}\gamma^{-4} - 3.8106 \\ & \times 10^{-10}\beta^{-6}\gamma^{-6})I^2 \\ & + (3.858019 \times 10^{-9}\beta^{-2}\gamma^{-2} - 1.667989 \\ & \times 10^{-10}\beta^{-4}\gamma^{-4} + 1.57955 \times 10^{-12}\beta^{-6}\gamma^{-6})I^3, \end{aligned} \tag{10}$$

which is considered valid for $\beta\gamma > 0.13$. I is the mean ionization potential of the target in units of eV and characterizes the rate of energy loss per unit path length. The shell correction applicable to the second situation takes into account the total ground-state electronic binding energy of the target atom [Leung, 1989; Leung, 1999]. This correction, however, does not provide any details about the role of the projectile charge in this situation [Weaver and Westphal, 2002].

Lindhard-Sørensen Correction

The Lindhard-Sørensen (LS) correction is a modern replacement for the corrections of Bloch [Bloch, 1933], Mott [Ahlen, 1980], and Ahlen [Ahlen, 1982], which are collectively referred to as the BMA group because of their common thread of development. This results in a more precise stopping power calculation in comparison to the separate treatment. The Bloch correction was derived by Felix Bloch in an investigation of the similarities and differences between classical and quantum mechanical range-energy calculations. The Mott correction addresses electron scattering off of highly charged nuclei. The Ahlen correction is applied to that of Bloch in regimes of both high charge and energy [Ahlen and Tarlé, 1983]. The Lindhard-Sørensen correction recovers the Bloch correction in the low-energy limit, while also incorporating Mott scattering in a relativistically correct manner [Lindhard and Sørensen, 1996]:

$$\Delta L_{\mathrm{LS}} = \sum_{k=1}^{\infty}\Big[\frac{k}{\eta^2}\frac{k-1}{2k-1}\sin^2(\delta_k - \delta_{k-1}) + \frac{k}{\eta^2}\frac{k+1}{2k+1}\sin^2(\delta_{-k} - \delta_{-k-1}) + \frac{k}{4k^2-1}\frac{1}{\gamma^2k^2+\eta^2} - \frac{1}{k}\Big] + \frac{\beta^2}{2}. \tag{11}$$

In Equation (11), $\eta = \alpha z/\beta$ is a dimensionless parameter with $\alpha = e^2/4\pi\epsilon_0\hbar c$ the fine structure constant; δ_k is the relativistic Coulomb phase shift; the index k is a parameterization of the angular momentum quantum numbers (including spin).

Finite Nuclear Size Correction

The finite nuclear size correction accounts for the physical size of atomic nuclei in the target medium [Datz et al., 1996]. This is possible because a precise mathematical description can be obtained for any spherically symmetric potential [Rose, 1961]. This correction appears as a modification to the Coulomb phase shift, δ_k, of Equation (11). This phase shift is a function of a parameter that provides a connection between the interior uniform (nuclear) spherical potential and the exterior Coulomb potential [Bhalla and Rose, 1962].

Barkas Correction

The Barkas effect goes back to the experimental observation of a 0.3% difference in the ranges of positive and negative pions as detected in nuclear emulsion [Smith et al., 1953]. This was interesting at the time because it could have indicated a difference in the masses of the particle and its antiparticle. Later tests attributed the effect to a difference in stopping powers—that of the negative pion is slightly lower—of the two particles and not to a mass difference [Barkas et al., 1963a; Barkas et al., 1963b; Heckman and Lindstrom, 1969]. More recent measurements confirm this effect by comparing the stopping powers of protons and antiprotons in the keV regime where the difference is more substantial [Medenwaldt et al., 1991]. The Barkas correction accounts for the effect of polarization within the target medium due to low-energy collisions between the projectile and distant electrons. Conceptually, if the projectile interacts with a harmonic oscillator, one obtains from simple dimensional considerations a correction factor of $3\pi z e^2 \omega / 2 m_\mathrm{e} v^3$ [Lindhard, 1976]. Operationally, however, it is recommended to multiply the leading term of the stopping logarithm, $\ln(2 m_\mathrm{e} v^2 / I)$, with the correction [Ashley et al., 1972; Ashley et al., 1973; Ashley et al., 1974; Jackson and McCarthy, 1972]:

$$L_\mathrm{Barkas} = 1 + \frac{2z}{\sqrt{Z}}[F(V)], \tag{12}$$

where $F(V) = 0.0019 \exp\{-2\ln(V/10)\}$ is a ratio of two integrals over a Thomas-Fermi model of the atom [Bohr, 1948; Bohr and Lindhard, 1954] and $V = \beta\gamma/\alpha\sqrt{Z}$ is the reduced momentum. The function $F(V)$ is not considered reliable below $V < 0.8$ [Jackson and McCarthy, 1972].

Finally, having obtained these corrections, Equation (2) reads:

$$\begin{aligned} \frac{dE}{dx} = \frac{n z^2 e^4}{4\pi\epsilon_0^2 m_\mathrm{e} v^2} \Bigg[& \left\{ \ln\left(\frac{2 m_\mathrm{e} v^2}{I}\right) + \Delta L_\mathrm{shell} \right\} L_\mathrm{Barkas} + \Delta L_\mathrm{LS} \\ & - \ln\left(1 - \frac{v^2}{c^2}\right) - \frac{v^2}{c^2} - \frac{\delta}{2} + 2\ln\gamma - 1 + \frac{1}{\gamma^2} \Bigg]. \end{aligned} \tag{13}$$

Equation (13), and the corrections it implements, is contained in a program given in Appendix B. The code also has the ability to implement other highly relativistic corrections not listed here. Figure 1, Figure 2, Figure 3, and Figure 4 illustrate the use of Equation (13) and the effect the various corrections described in this section have on stopping power. Each curve corresponds to a plot of Equation (1) plus the listed correction.

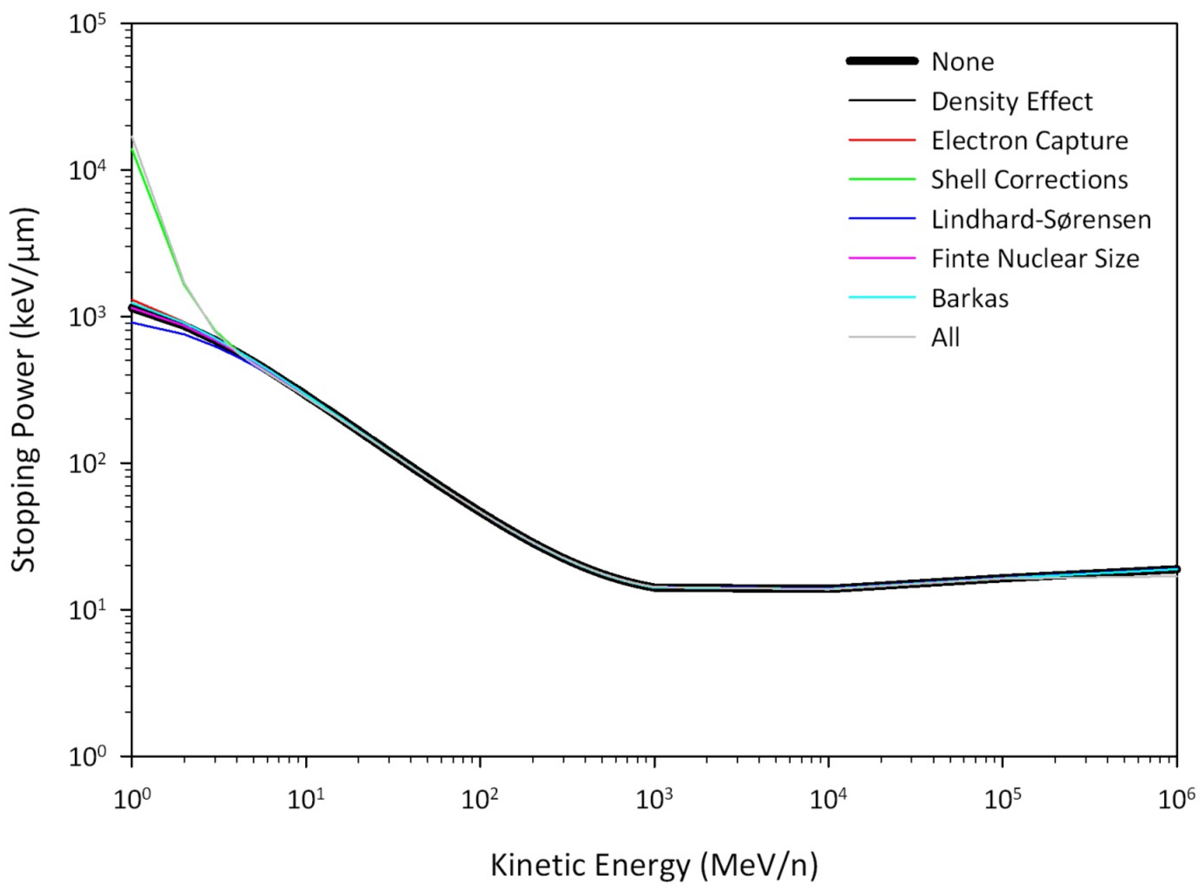

Figure 1 Stopping power as a function of projectile kinetic energy for ^{16}O in a water target.

Figure 1 shows stopping power in keV/μm of ^{16}O in water as a function of projectile kinetic energy in MeV/nucleon. The family of curves depicted in this plot demonstrates the relative effect a given correction has on the stopping power of the projectile. Compared to the "bare" Bethe-Bloch formula, Equation (1), the Lindhard-Sørensen correction tends to decrease the stopping power by a small amount below energies of about 4 MeV/n. Conversely, shell corrections increase the stopping power substantially below this limit, which is comparable to having all the listed corrections switched on. This suggests that shell corrections are important below approximately 4 MeV/n when a "light" ion (^{16}O) penetrates a "light" target (water). The other corrections in Figure 1 seem to have little effect overall.

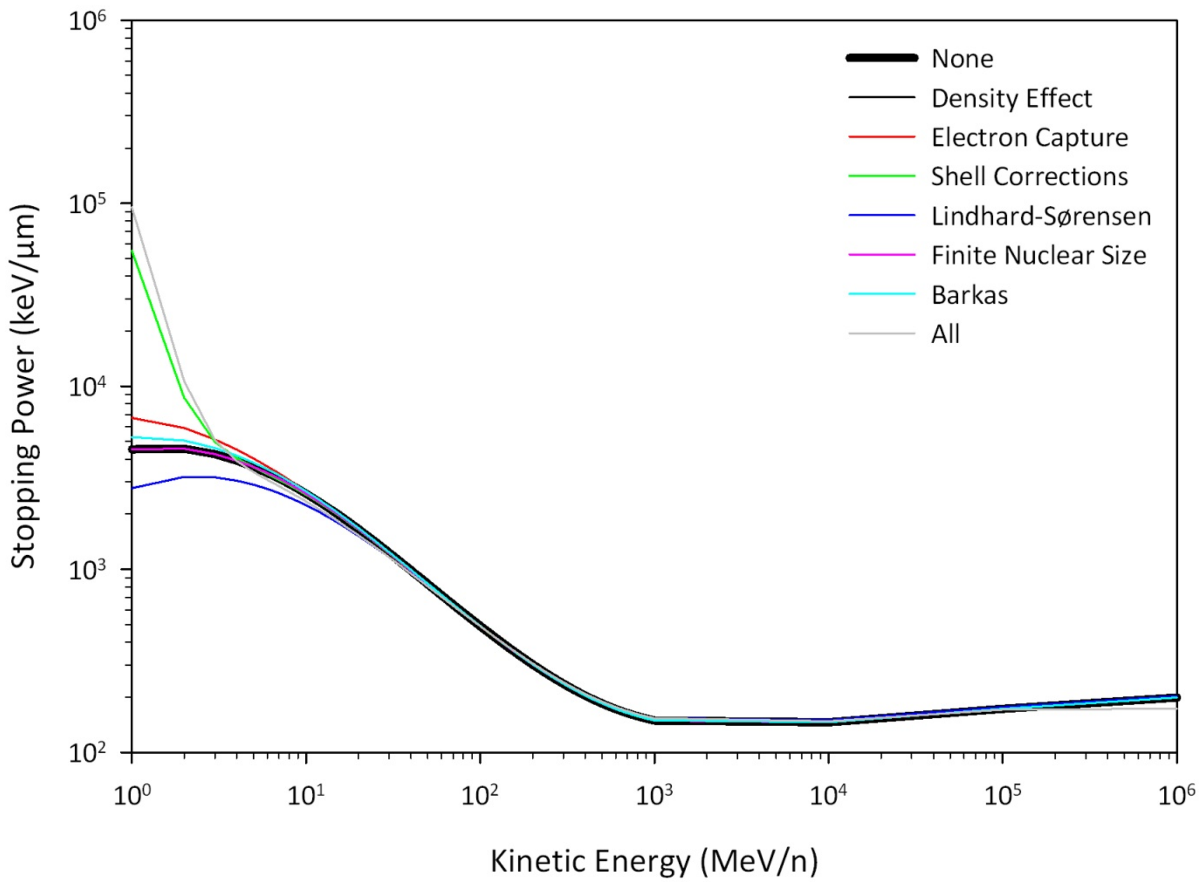

Figure 2 Stopping power as a function of projectile kinetic energy for ^{56}Fe in a water target.

Figure 2 shows stopping power in keV/µm of ^{56}Fe in water as a function of projectile kinetic energy in MeV/nucleon. The Lindhard-Sørensen correction decreases the stopping power below energies of about 20 MeV/n. The Barkas correction increases the stopping power only slightly at kinetic energies below roughly 3 MeV/n, with electron capture contributing more below a limit of 6 MeV/n. As seen in Figure 1, shell corrections provide the greatest increase in stopping power when compared to the curve where all listed corrections are turned on. This indicates that shell corrections are important below approximately 4-5 MeV/n when a "heavy" ion (^{56}Fe) penetrates a "light" target (water). The density effect and finite nuclear size corrections in Figure 2 apparently do not influence stopping power to any large degree.

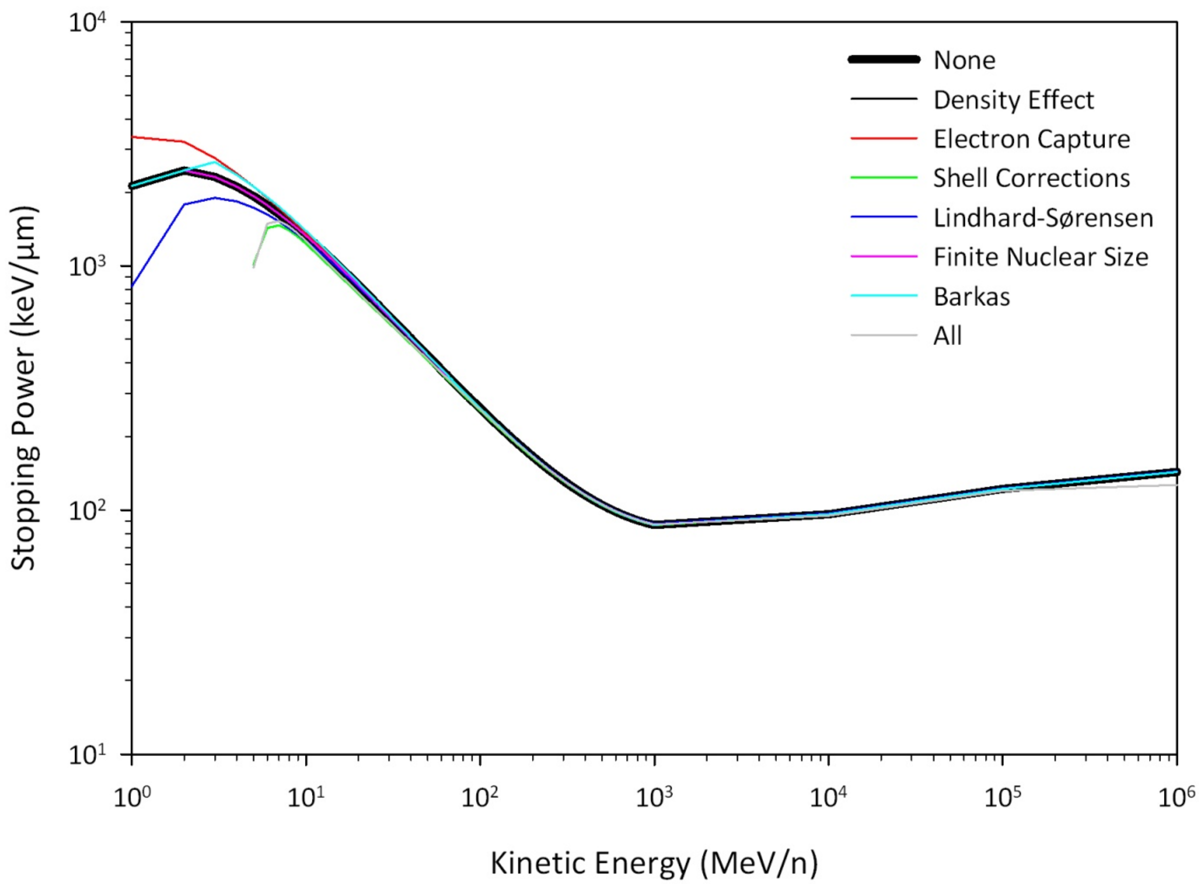

Figure 3 Stopping power as a function of projectile kinetic energy for ^{16}O in a lead target.

Figure 3 shows stopping power in keV/µm of ^{16}O in lead as a function of projectile kinetic energy in MeV/nucleon. Electron capture increases stopping power the most below about 7 MeV/n; interestingly, the Barkas correction only seems to take effect between approximately 2 and 7 MeV/n. The Lindhard-Sørensen correction decreases the stopping power more than shell corrections below about 8 MeV/n. Once again the curve with shell corrections implemented and the curve with all the listed corrections switched on are similar to one another. This suggests that shell corrections are important below approximately 10 MeV/n when a "light" ion (^{16}O) penetrates a "heavy" target (lead). The density effect and finite nuclear size corrections in Figure 3 do not affect stopping power appreciably.

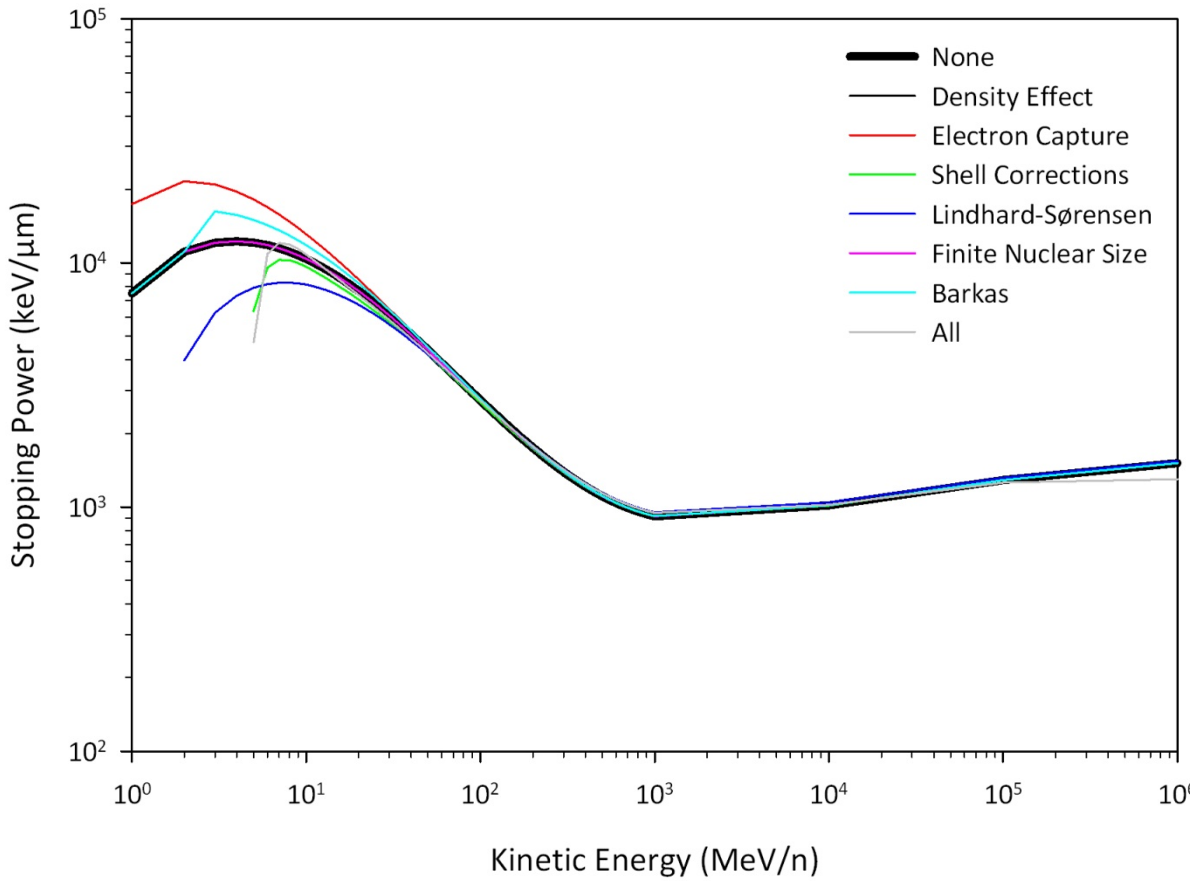

Figure 4 Stopping power as a function of projectile kinetic energy for ^{56}Fe in a lead target.

Figure 4 shows stopping power in keV/µm of ^{56}Fe in lead as a function of projectile kinetic energy in MeV/nucleon. Electron capture shows the most substantial increase in stopping power below about 30 MeV/n, with the Barkas correction taking effect between approximately 2 and 30 MeV/n.

Similar to Figure 3, the Lindhard-Sørensen correction presents the most substantial decrease in stopping power below approximately 40 MeV/n. Again, shell corrections seem to influence the behavior of stopping power the most. Shell corrections seem to be important below approximately 40 MeV/n when a "heavy" ion (^{56}Fe) penetrates a "heavy" target (lead). The density effect and finite nuclear size corrections once again do not affect stopping power appreciably.

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